A Novel Model Adaptation Method for Multivariate Statistical Process Control

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1. Introduction

Process monitoring has been widely employed to guarantee process safety and product quality and to identify state of process (Rosen & Lennox, 2001). Process monitoring is required both to detect process changes as early as possible and to reduce the number of false alarms (Kano & Hasebe & Hashimoto & Ohno, 2002). Multivariate statistical process control (MSPC) based on Principal component analysis have widely applied to resolve these hot issues to process monitoring. However, process changes such as mode changes and disturbances occur very frequently due to demand variation of products, fluctuations in raw materials, and fluctuations in utility prices in real industrial plants. The MSPC monitoring based on PCA is difficult to apply to process with non-stationary and time-varying behavior.

Wold et al. (1994) and Gallagher & Wise & Butler & White & Barna (1997) have introduced the use of EWMA, EWMC, and EWM-PCA. It is hard to reflect process changes well because the approach uniformly applies the exponentially decreasing weights without any considerations to process change. Hwang & Han (1999), Chen & Liu (2000), and Choi & Park & Lee (2004) have introduced model library based methods. They used the classified models with their corresponding modes. It is comprised of two steps; (i) clustering as operating modes, and (ii) local PCA monitoring. These methods have a factor to consider: operating modes are not fixed. Therefore, model library should be still updated continuously according to operating modes newly generate. Li & Yue & & Valle-Cervantes & Qin (2000) presented monitoring strategy calculating the model recursively with a moving window. Moving window based recursive method carries out *blind update* which means continuous update without identifying a type of the process changes. It can be doubtful that model is satisfactorily updated due to disturbance adaptation.

This paper proposes a novel monitoring methodology for the process which includes frequent operating mode changes. The core idea of the proposed approach is (i) to combine process knowledge for detection of mode change with statistical indices in order to seek an

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update starting point. It is more useful way to search optimal update points due to the fact that decision with physical meanings would avoid wrong judgment by biased parameter estimation, (ii) to introduce new index to reflect process changes well. It means exponentially decreasing weights are applied by not constant but variables and (iii) to stop model update keeps from unnecessary model updating and disturbance adapting.

2. The proposed approach

Figure 1 shows overview of the proposed approach. Approach consists of (i) detection of process change by two indices, the Hotelling's T^2 and the squared prediction error (SPE), (ii) Identification of process change either mode change or disturbance, (iii) Removal of disturbance data to keep from adapting of disturbance, and (iv) Update model using flexible forgetting factor and detect steady-states to stop model adaptation

2.1 Detection of process changes

Process changes generally include operating mode changes, start-up or shut-down, and disturbances. It is that start-up or shut-down is easy to detect. This study treats the detection of mode changes and disturbances. Abnormal situation will cause at least one of T^2 and SPE values to deviate from the control limits. Data matrix X can be approximated using loading matrix P_k, score matrix T_k, and a residual matrix E. Each matrix, loading matrix and score matrix can be divided into loading vector p_k and score vector t_k.

$$X = t_1 p_1^T + t_2 p_2^T + t_3 p_3^T + \cdots + t_k p_k^T + E = T_k P_k^T + E \quad (1)$$

$$X_i = \begin{bmatrix} x_{\text{i-1}} \\ x_{\text{i}} \end{bmatrix} \quad (2)$$

$$\mathrm{x}_{\mathrm{i}} = R_i x_{\mathrm{i}} + (1 - R_i) x_{\text{i-1}} \quad (3)$$

$$T_i^2 = \mathrm{x}_{\mathrm{i}} P_k \Lambda_i^{-1} P_k \mathrm{x}_{\mathrm{i}}^{\mathrm{T}} \quad (4)$$

$$Q_i = \mathrm{x}_{\mathrm{i}} (I - P_k P_k^T) \mathrm{x}_{\mathrm{i}}^{\mathrm{T}} \quad (5)$$

where X_i is mean centered vector combining $(\text{i-1})_{\text{th}}$ data set with i_{th} data set. R_i is a forgetting factor. Λ_i is a diagonal matrix containing the eigenvalues, I is an identity matrix, and k is a number of principal components. T_i^2 shows a measure of the variation within the PCA model for each observation. Q_i shows a measure of how well the new observation is described by the PCA model. Control limits are given by

$$T_i^2 > \frac{k(N^2 - 1)}{N(N - k)} F_{k, N-k, \alpha} \quad (6)$$

$$Q_i > \left(\frac{\sigma^2}{2\mu}\right)\chi^2_{\frac{2\mu^2}{\sigma^2},\alpha} \tag{7}$$

where N is a number of observations on the model training set, and $F_{k,N-k,\alpha}$ is the critical value of the F-distribution with $k, N-k$ degree of freedom at the confidence region α. μ and σ is a sample mean and standard deviation on the model training set, and $\chi^2_{\frac{2\mu^2}{\sigma^2},\alpha}$ is the critical value of the Chi-squared variable with $\frac{2\mu^2}{\sigma^2}$ degree of freedom at the significant level α. These points are considered as candidates of time points for model update.

2.2 Identification of process changes

Process changes tend to move the process operating point radically out in different directions in score plot. However, the process changes will confirm either mode changes or disturbances after process changes occur. A solution to the problem lies in using a new method for real-time identification of process changes.

If process change is detected, if-then rule begin to identify process change whether current change is mode change or not. If mode change occurs, variables of roots cause should exceed control limits. If-then rule for detection is simply shown as

IF {change of $factor_i$ and change of effect of causal $factor_i$ and identification of no disturbance ($factor_i$)}, THEN operating mode change by $factor_i$ (8)

Each operating mode change rule by equation (8) is (i) set point change of outlet temperature, (ii) change of API, (iii) change of correlation between feed flowrate and air flowrate, and (iv) change of used burners' number.

2.3 Model update

Steps for model update consist of (i) outlier removal, (ii) update the model using flexible forgetting factor, and stop adaptation through detecting of steady-states.

2.3.1 Outlier removal

Outlier is deviated significantly out of normal region due to start-up or shut-down, sensor malfunction, process disturbances, instrument degradation, and human-related errors (Liu & Shah & Jiang, 2004). Therefore, outlier data should be just isolated due to having unnecessary information. Therefore, this helps keep from adapting insignificant information, reduces the number of update as well as false alarms.

2.3.2 Start update and stop adaptation

The main steps are as follows:

(i) Update according to each quantitative magnitude of process change. For example, if process of i_{th} time suddenly and frequently changes, history data of $(i-1)_{th}$ and $(i-2)_{th}$ times would have relatively little influent information as compared against less suddenly and frequently changes. To cope with this problem, flexible forgetting factor has been introduced. That is, forgetting factor, R_i is applied by not constant but variable according to quantitative magnitude of process change. Flexible forgetting factor is calculated from value of D (Kano & Hasebe & Hashimoto & Ohno, 2002). Value of D is given by

$$Y_i = \sqrt{\frac{N_i - 1}{N - 1}} X_i P_o \Lambda^{-\frac{1}{2}} \tag{9}$$

$$D_i = \frac{4}{k} \sum_{j=1}^{k} (\lambda_i - 0.5)^2 \tag{10}$$

where N_i is the number of i[th] data set samples. P_o is orthogonal matrix of eigenvector. λ_i is eigenvalues of Y_i's covariance matrices. D_i is to quantitatively evaluate the difference of covariance between (i-1)[th] data set and i[th] data set.

Model update carries out using equation (11) and (12) when process change is identified as mode change by if-then rule.

$$T_{i+1}^2 = D_i T_i^2 + (1 - D_i) T_{i-1}^2 \tag{11}$$

$$Q_{i+1} = D_i Q_i + (1 - D_i) Q_{i-1} \tag{12}$$

where D_i is used to flexible forgetting factor.

(ii) Define model adaptation stopping point. Generally, if the process is assumed to be in control, any action is not necessary at all. A solution is what carries out monitoring without model update till next mode change will happen. Steady-state is where process change does not happen and generated process data would be stationary and time-invarying condition. In order to define criterion for stop model adaptation, it is assumed that D is normal distribution. Almost all operations condition should comprise from $\mu - 3\sigma$ to $\mu + 3\sigma$. Therefore, steady-states is considered D is smaller than $\mu - 3\sigma$. Criteria of D are given by

$D \sim N(\mu, \sigma^2)$ and $\mu - 3\sigma \le D \le \mu + 3\sigma$, then $D < \mu - 3\sigma$ (13)

The main steps for model update with the proposed approach are summarized in Table 1.

3. RESULTS AND DISCUSSION

3.1 Process description

An industrial fired heater is applied to demonstrate validity of the proposed approach. Burners generate the heat by the combustion of fuel. Oil and gas are consumed as fuel to heat feeding oil. The test data are gathered 2 months. Window-size is 3 days and block-size is 6 hours.

3.2 Monitoring with the proposed approach

Mean value of D is 0.4729 and standard deviation of D is 0.005 respectively.

Therefore, a criterion of D is smaller than 0.4579. Figure 1 shows the result of monitoring during 2 months.

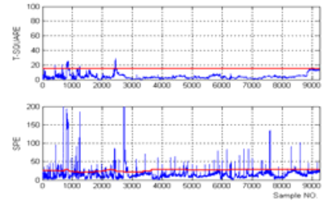
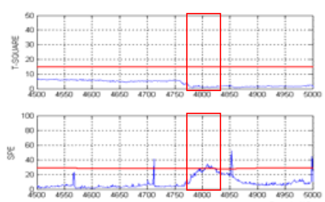


Figure 1. Monitoring result of the proposed approach

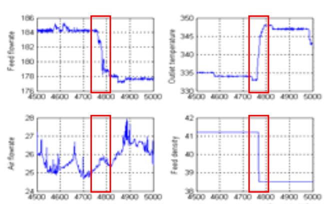
There are 39 times mode changes and model update executes 52 times by model update criteria. As shown in Figure 2, the proposed approach detects mode change on fast when mode change occurs. Mode change happens around 4750 sample number. Improving model accuracy becomes clear due to the evidence that four variables exceed the control limits with their correlation and causality. Figure 3 shows that disturbance goes through from 4455 to 4465. Model update after isolation of disturbance can almost completely rule out the possibility regarding disturbance adaptation.

3.3 Comparison of monitoring between the proposed approach and recursive PCA

Figure 4 shows the result of recursive approach during about 2 months. It shows clearly that Figure 4, the result of recursive PCA monitoring, has lots of false alarms than Figure 1, that of the proposed approach from the model accuracy point of view. Efficiency of the proposed approach shows in Figure 5. The number of model updates from recursive PCA is 29. On the contrary, that model update does not carry out ranging roughly from 5350 to 5500 and other points is why the number of model update from the proposed approach is just 9. Table 1 summarized that the proposed approach shows definitely better performance.

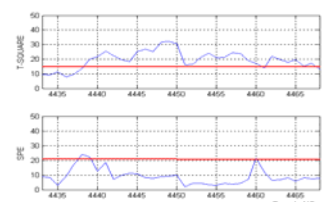


(a)

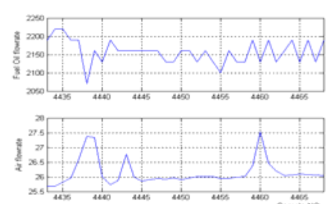


(b)

Figure 2. Detection of mode change with the proposed approach: (a) The proposed approach, (b) Variables for mode detection



(a)



(b)

Figure 3. Disturbance detection with the proposed approach: (a) The proposed approach, (b) Variables for disturbance detection

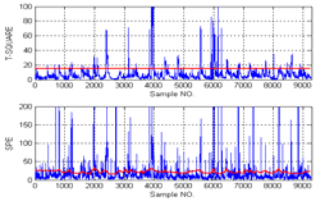
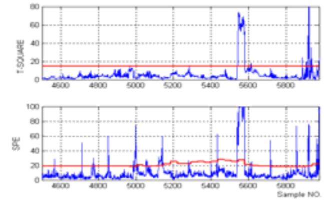
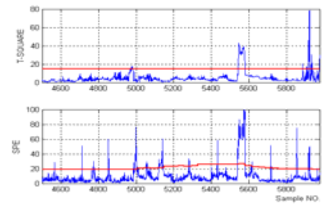


Figure 4. Monitoring result of recursive PCA



(a)



(b)

Figure 5. Comparison of the number of update for recursive PCA with that of the proposed approach: (a) Recursive PCA, (b) The proposed approach

		Recursive PCA	The proposed approach
Normal	Accept (units)	7171	8475
(8823)	Reject (units)	1649	348
	Type I error	0.2287	0.0411
Abnormal	Accept (units)	32	0
(127)	Reject (units)	95	127
	Type II error	0.3368	0
Efficiency	Number of update	245	52

Table 1. Overall results

4. Conclusion

Improved performance is known by following facts: (a) whether it decreases both type I error and type II error or not, and (b) whether it execute less the number of model update or not. The proposed approach lessened type I error and type II error and the number of update as well under frequent and sudden process change because to fill up the demand to end-user and the optimal distribution to inventory. The proposed approach uses any process knowledge to know current status so that it can be applicable to wide operation modes and various process conditions without dividing local monitoring. As the result of lack of identifying current status, recursive PCA monitoring leads such shortcomings as adapt disturbances and unnecessarily updates at steady-states. Besides, the problem towards slow confirmation of process changes is serious that not only does model update execute at unsuitable time but also model adaptation becomes late.

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